BEST PRACTICES FOR REDUCTION OF UNCERTAINTY IN CFD RESULTS (INVITED)

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Abstract

This paper describes a proposed best-practices system that will present expert knowledge in the use of CFD. The best-practices system will include specific guidelines to assist the user in problem definition, input preparation, grid generation, code selection, parameter specification, and results interpretation. The goal of the system is to assist all CFD users in obtaining high quality CFD solutions with reduced uncertainty and at lower cost for a wide range of flow problems. The best-practices system will be implemented as a software product which includes an expert system made up of knowledge databases of expert information with specific guidelines for individual codes and algorithms. The process of acquiring expert knowledge is discussed, and help from the CFD community is solicited. Benefits and challenges associated with this project are examined.

Introduction

A common research goal in CFD is to make CFD less of an "art" and more of a "science." The artistry of CFD involves the expertise and diligence of the CFD engineers controlling the many details that go into a CFD calculation. These skills typically take many years of schooling and experience to acquire. An effective approach to furthering the science of CFD is to provide specific guidance and a checklist of properties to verify in a solution. This information will be useful to the expert and nonexpert alike, to ensure that all reasonable steps have been taken to ensure the accuracy of a CFD solution.

For purposes of initiating this discussion, the concept of “Best Practices” will be defined as a set of specific guidelines for CFD users to assist in grid generation, the selection of parameters that control the CFD code execution, the assessment of the resulting solution, and diagnosing abnormal results. The best-practices guidelines will be a practical set of instructions and a check list for CFD users, and it will provide a tutorial function for novice users or experienced users unfamiliar with a specific code. The software approach to accomplish best practices for CFD analyses is outlined in this paper. Another important intent of these descriptions is to create a forum for discussion in the CFD community to supplement and improve this initial approach.

Motivation

CFD plays an essential role in the design and analysis of advanced aerospace vehicles, and uncertainties in CFD results affect the performance of aerospace products. In the past two decades, CFD has evolved from a research topic to an integral tool in aerospace design. Many aircraft are designed on the computer and then validated in wind tunnel and flight tests; however, uncertainties in CFD analyses limit the ability to optimize aircraft performance. Shape optimization of aircraft via a traditional "cut-and-try" physical process has always been expensive, and it will be required less often as uncertainties in CFD results diminish.

The reliability and cost of performing CFD analyses are also important issues in product design, as reliance on CFD increases. Any time and cost savings in this process will lead directly to a reduction in costs of the design and development program; therefore, it is important that the use of the CFD tools become more efficient. To do this, unnecessary CFD runs must be eliminated, errors need to be minimized as efficiently as possible, and mistakes of the past cannot be repeated.

The problem of interest and the flow physics to be modeled determine the CFD approach that the user must choose to obtain reliable and accurate analyses. CFD is called on to model a wide range of flow problems. The required output from a CFD analysis varies from simple forces and moments to detailed turbulent, reacting flow structures. Each flow regime may require its own special approach to ensure satisfactory results, and each CFD algorithm and code may have its own individual requirements.

The long-term goal of "turn-key" CFD methods remains elusive, and CFD is heavily dependent on CFD engineers to regulate the many parameters that govern a CFD analysis. CFD users are generally required to (1) anticipate flow characteristics, (2) select appropriate modeling technology (boundary conditions, turbulence model, shock capturing, etc.), (3) construct an appropriate grid, and (4) ensure that the solution is converged in all senses. Iteration on some steps may be required. While many tools exist to assist the user in these steps, final decisions depend on human expertise and diligence, subject to cost and schedule constraints. This process has many opportunities for poor decisions that introduce errors in the CFD solution. The concept of best practices is primarily intended to assist all users in making decisions that lead to consistently good CFD results.

Background

It is recognized that the user has a critical role in current CFD processes and that the quality of CFD results is subject to significant variability. The application of and search for best practices in CFD is not new. The concept of best practices can take many different forms, all of which are useful, but none of which are complete in themselves. Some recent examples of best practices are described below.

- Chan et al at NASA discuss a best-practices process for overset grid generation.[2] This reference includes nearly ninety specific recommendations and guidelines for the preparation of overset grids to achieve successful CFD solutions for a variety of flow problems.
- Another approach to best practices for grid generation is under development for the GRIDGEN software.[3] In this effort, an automatic meshing approach will be included to eliminate many of the common problems that occur in the grid development process.
- The ERCOFTAC Best Practices Guidelines[4] is a 94-page printed document with many rules and procedures that require significant user effort to implement. This work also includes a discussion of the selection of turbulence models.
- A set of practical guidelines for the application of CFD methods for hydrodynamic flows in the marine industry is available.[5] This work is presented in a manner similar to the ERCOFTAC document.
- An effort to collect and disseminate expert knowledge in CFD for more effective industrial applications in Europe is underway in the QNET-CFD thematic network.[6]
- The work by Roache describes specific procedures for the correct use of grid convergence studies to assess grid dependence.[7]
- The WIND solver includes algorithms that evaluate grid quality in every CFD run and notifies the users of potential problems.[8]

Other work has implemented best-practices concepts as algorithmic tools to be used in conjunction with CFD analyses. For example, there have been recent efforts to develop analysis codes that quantify the effects of truncation errors on a CFD solution.[9] Others are working toward intelligent solution-adaptive gridding via solutions of the adjoint equation.[10]

All of these methods and approaches provide important information for using CFD software in the most appropriate manner. They also indicate a perceived need for best practices. However, many of these approaches require a skilled practitioner to interpret the results and implement corrective actions. Many problems can be traced to inexperienced users producing results with software they do not understand.[1]

A recent exercise illustrates the need for best practices for CFD analyses. The AIAA Drag Prediction Workshop (DPW) involved many CFD and aerodynamics groups in the United States and Europe for the purpose of analyzing a single, simple wing/body model of a modern transonic transport aircraft. The DLR-F4 wing-body configuration was chosen for the study because it had been tested in multiple tunnels, and there is high confidence in the quality and accuracy of the data.[11,12] These data have been used in other studies, so there is a significant history of study on this configuration.[13] For the DPW, a total of 35 solutions were computed with 14 different CFD codes. Multiple turbulence models were used, structured and unstructured grid topologies were used, and 21 solutions used exactly the same grids. The variation in the CFD results was 40 times the value sought for aerodynamic design and more than five times the variation seen in the experimental data. These variations exist even when some of the known contributors to uncertainty, like turbulence modeling, were eliminated.[14,15]

Many of the CFD experts involved in the DPW noted that details of the calculations were not treated with sufficient care, generally because of time and budget constraints. Other researchers spent the extra time required to better understand some of the issues affecting solution errors; for example, several levels of mesh refinement at the thick trailing edge were required before grid dependence was essentially eliminated. Time and budget constraints are the norm in CFD applications; therefore, there is a need for best practices to assist the user in achieving the best solutions possible given these restrictions.

Challenges

The development of specific best-practices guidelines with broad applicability is challenging for many reasons, a few of which are given here.

- Best practices are intended to encapsulate extensive knowledge that typically requires years of education and work experience to acquire. Other best-practices guides are lengthy printed documents and do not have specific guidelines for individual codes and algorithm options.
- Best practices cannot be static. CFD algorithms continue to evolve, new codes are written, and individuals may customize CFD solvers for specific needs. Individual organizations may have proprietary or esoteric-domain expertise they wish to store in best practices form.
- There are many CFD algorithms, solvers, and codes, each with potentially different requirements for best usage. A broadly useful best-practices system must handle both generic and code-specific information.
- A best-practices guide that is large enough to contain all the above information must have computerized search and cross-reference capabilities.
- For some issues, actual best practices do not exist. Users have “accepted” or “current” practices that seem to be adequate and are widely used. However, a best-practices system must acknowledge its limitations. This requires the distinction between best practices based on sound mathematics and observed behavior, and those techniques used without a full understanding of why they produce acceptable results.
- Some information needed for specific best practices may be difficult to obtain. Many errors in CFD depend on mesh spacing or stretching in some algebraic manner. Rather than specifying absolute target values for grid properties, scalings and typical reference values are required. (E.g., the error in skin friction scales on $(y^+_{min})^2$ and it is about 1% for some value of y^+, for a given turbulence model.) Experts may have intuition about these traits of CFD, but it is difficult to provide specific knowledge to share with others.

The issues raised above give a sample of the problems that must be resolved to provide a truly comprehensive best-practices system.

Technical Direction

The authors envision a system of best practices that will provide state-of-the-art capability for CFD analyses to all levels of users. The core of best practices is the knowledge and experiences of successful CFD developers and users. This expert information will provide the guidelines for successful set-up and execution of CFD calculations, problem diagnosis, and remedy of problems.

The proposed system will be based on the approach developed for an integrated aerodynamics design and analysis system called LVX (Launch Vehicle eXpert).[16,17] This system incorporates expert knowledge, historical design guidelines, corporate memory, and a documents database into a knowledge-based system. The existing software with searchable and related databases and the knowledge acquisition process developed to populate the databases provide an approach to best practices that meets the initial requirements. It will make the best practices techniques and experiences available to all levels of users and provide a means for continual upgrades and maintenance. The following sections discuss the proposed system in greater detail in an effort to elicit constructive comments and criticisms from the CFD user community.

Objectives

The objective is to guide the development of best practices so that they can be broadly applied by users interested in reducing the time and cost associated with CFD use and also improving the accuracy and reducing the uncertainty of CFD results. Some of the characteristics of best practices must include the following:

- Demonstrate ease of use for all levels of users.
- Provide an intuitive process for general acceptance by the CFD community.
- Provide information appropriate for all CFD users to achieve more reliable CFD results with less effort.
- Provide a comprehensive compendium of procedures and expertise that should be followed to get the required accuracy from CFD.
- Apply to the different ways that people and organizations use CFD.
- Evolve with advancements in CFD algorithms and codes.
- Choose a framework for best practices applicable to all algorithms and solvers that developers and/or users are willing to support.
- Permit individual users to customize details of best practices to support specific needs and provide for proprietary versions of the system.
- Provide a self-critical system by noting the relative confidence in specific guidelines and characterizing the aspects of CFD practices that are poorly understood.
- Provide the flexibility to evolve into a future system which may require highly automated CFD quality assurance algorithms, including automatic grid generation and solution interrogation algorithms.

Approach

The planned approach to best practices is based on the authors' anticipation of its use by a community of CFD users with a wide range of experience and needs. The techniques and information provided to the user, either in response to questions submitted or to selections made during input preparation, will come from the expert knowledge base of best practices. The proposed approach to implement best practices is based on recent experience with a similar system developed for missile and launch vehicle aerodynamic design (LVX).[16,17]

LVX is built around an expert knowledge database which includes design rules and engineering rules-of-thumb. It includes knowledge gained from experience on aerospace programs, as well as information from published guidelines, design tutorials, and position papers. Valuable information was obtained from historical data reports and key interviews with active and retired experts from NASA and industry. All of the design rules and comments gleaned from the multitude of sources are included in the database with links to design information associated with specific configurations and to published documents.

The LVX process is illustrated in Fig. 1.

The related knowledge databases in LVX incorporate:

- Corporate memory and experience
- Expert knowledge relating to aerodynamics of missiles and launch vehicles
- Historical information
- Pictures and drawings of existing designs
- References to published reports (2,600 citations)
- Detailed information on codes and computational options
- Specific code critiques and suggestions for appropriate prediction methods
- Aerodynamic analysis codes for preliminary estimates
- Experimental and computational data

The searchable expert-knowledge databases are linked together by common and related topics. The user has access to the information through a search feature, and the results of a specific search include direct links to related information. Each of these databases can be used to represent some key aspect of the best-practices system, and the existing LVX software framework can be applied directly to the proposed system.

As noted above, the expert knowledge must be expanded and modified as new information and experiences dictate; consequently, LVX has an update procedure included. Initially, the developers of the system will accomplish and test all the updates to the system using information provided by CFD users, but after the system matures, it may be possible for the users to update the system via a web-based approach. If this is accomplished, some means to screen and evaluate the information included is required to maintain the high quality of the information in the system. It will also be possible to include dissenting opinions in those areas where controversy exists.

In addition to the use of the existing LVX software, some of the more intangible results of the LVX development work will provide valuable insight for the proposed best-practices system. The lessons learned during the system development, particularly in the knowledge acquisition process, will be directly applicable to CFD best practices. For example, some expert information will be obtained through an interview process, but it is critical that the interviewer not bias the information obtained with their own experiences and opinions. It is also important to be aware of proprietary or other sensitive information during the knowledge-acquisition process. Finally, the information obtained during individual interviews must be verified for accuracy and reliability before inclusion into the knowledge databases.

Framework

The structure of the initial best-practices system will be based on the techniques, processes, and procedures used in the LVX system. The selection of available and proven software will lead to a working best-practices system in the shortest possible time. However, even though the basic framework of LVX will be unchanged, a number of details will require change to adapt the process to CFD information.

A hierarchical keyword structure is used to organize the knowledge stored in the databases. Each node in the hierarchy is represented by a keyword associated with a topic. This model allows the information stored to be linked in a logical fashion, which assists in both the knowledge acquisition and the knowledge retrieval mechanism. There are more than four hundred keywords in the current LVX hierarchy, and the user can add additional keywords as needed.

For purposes of initiating the discussion on best practices, a high-level hierarchy of keywords is shown in Fig. 2. This is not a complete list, nor is the order shown the definitive and final hierarchy. This specific top-level keyword outline is shown to begin the discussion of important topics which must be included.

The hierarchy is a way to organize the information in the databases so that it is easily accessible for editing and maintenance purposes. It is important that the keyword list be comprehensive and as complete as possible; however, the actual position or location of the topics in the hierarchy is not critical in the LVX system. There are many links and connections between keywords at all levels in the hierarchy so that the interdependence between topics is maintained without regard to their physical location in the hierarchy.

Extensions of two specific topics, Governing Equations and Grid Generation, are shown in Figs. 3 and 4, respectively. These extensions illustrate a way to sort the expert information into the proper context, and they also provide a convenient means to identify holes in the expert information databases. Note that each level of the hierarchy shown in these figures can be further subdivided and extended as needed when the detailed information is sorted and organized.

Example

An example of the type of specific information that will be maintained in the database is shown below. In the actual use of the best-practices system, the information would be shown along with links to the technical references, justification information, and other supporting and even conflicting information.

As learned in the LVX work, it is important that the attribution of the knowledge be maintained to track the evolution and application of the best practices. Much of the following information is taken directly from the references, and where possible, appropriate credit is noted. Some specific expert knowledge for two topics follows.

- Low Reynolds number turbulence models
  - Two-equation turbulence models often recommend a wall spacing with y^+-values less than one, where y^+ is the nondimensional turbulent distance.[2]
  - One-equation turbulence models require a wall spacing given by y^+ approximately equal to one.[2]
  - Typically, 20 to 30 points in the boundary layer is considered good resolution.[2]
  - Depending on the Reynolds number, ensure that there are between five and ten mesh points between the wall and y^+ equals 20, which likely results in thirty to sixty points in the boundary layer for adequate boundary-layer resolution.[4]

- Wall functions
  - A significantly larger wall spacing can be used corresponding to y^+ between 35 and 100.[2]

- Check the lower limit of y^+. The meshing should be arranged so that the values of y^+ at wall adjacent integration points is only slightly above the recommended lower limit given by the code developers, typically between 20 and 30.[4]
- Check the upper limit on y^+. In the case of moderate Reynolds number, where the boundary layer only extends to y^+ of 300 to 500, there is no chance of accurately resolving the boundary layer if the first integration point is placed at a location with the value of y^+ of 100.[4]
- Check the resolution of the boundary layer. Adequate boundary layer resolution requires at least 8-10 points in the layer.[4]

These examples illustrate in an abbreviated manner the type of specific information which will be available to the CFD user; however, they also illustrate some of the basic problems that must be addressed by best practices. Ignoring the fact that the recommendations do not specify a specific code or physical problem, there are two problems with the examples. First, they do not address the uncertainty in the skin friction associated with the chosen y^+ values, and second, they do not address how uncertainty scales with y^+. This is the type of extended information which must be included in the expert knowledge provided to the user.

Discussion and Conclusions

This discussion of best practices for CFD users has been intended as a position paper for a proposed system, and the hope is that the CFD community will respond with suggestions and comments as well as support for the project by sharing the accumulation of expert knowledge. A proven knowledge-based system approach has been selected for use as the shell around which the best-practices tool will be organized to minimize development effort and time.

A number of implementation options are under consideration. The initial working best-practices method will be based on state-of-the-art knowledge and successful procedures as determined from the CFD developer and user community. Participation will be open to any in the developer and user community who are willing to share their experiences and information for the benefit of other users. A general open version will be developed first to test and evaluate the approach and usefulness, and this version will be made available publicly either through publication or electronic means to all interested parties. The users and organizations who participate by sharing knowledge and information will be shown some preferential treatment by receiving more frequent updates and evolving versions of the software system.

As learned during the LVX development, proprietary versions for specific user organizations may be required because of the need to include sensitive and restricted information. The details on the development of these specific versions of the system are to be determined when the need arises. One possible approach is for these versions to be available on a subscription basis to cover the added costs associated with including specific expert knowledge. This approach is currently available for the LVX software.

Continued experience and advances in CFD experience will add to the general knowledge base, and provision must be made to maintain and upgrade the system. The details of the specific process to identify new knowledge for inclusion into best practices are yet to be determined. This includes the process of evaluation of the quality of the information selected for best practices, how it is attributed, and how it is verified.

Once best practices for CFD are understood and accepted by the user community, automation should be considered. However, no matter what level of automation of best practices is ultimately achieved, the user must always be informed about decisions made, have access to the reasoning and justification for any recommendations, and have the ability to override any changes.

Acknowledgements

The authors wish to thank Dr. Michael J. Hemsch and Dr. James M. Luckring of NASA Langley Research Center for their constructive comments on this paper and their support for the best-practices concept.

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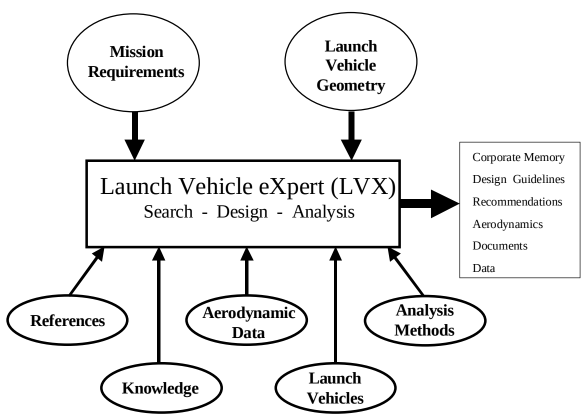

Figure 1.- LVX overview.

Figure 2.- Best Practices Top-Level Hierarchy

1.0 Physical Problem Definition
- 1.1 General Comments
- 1.2 Configuration Definition
- 1.3 Key Flow Regimes, Flow Physics, etc
- 1.4 Results Needed

2.0 Mathematical Problem Definition
- 2.1 Governing Equations
  - 2.1.1 General Comments
  - 2.1.2 Panel Methods
  - 2.1.3 Transonic Small Disturbance (TSD)
  - 2.1.4 Potential
  - 2.1.5 Euler
  - 2.1.6 Reynolds Averaged Navier-Stokes (RANS)
  - 2.1.7 Parabolized Navier-Stokes (PNS)
  - 2.1.8 Unsteady Reynolds Averaged Navier-Stokes (URANS)
  - 2.1.9 Detached Eddy Simulation (DES)
  - 2.1.10 Large Eddy Simulation (LES)
  - 2.1.11 Direct Numerical Simulation (DNS)
  - 2.1.12 Direct Simulation-Monte Carlo (DSMC)
- 2.2 Physical Modeling
  - 2.2.1 Transition and Turbulence Modeling
  - 2.2.2 Gas and Chemistry Modeling (combustion, plasmas, MHD, etc.)
  - 2.2.3 Multi-Phase Modeling
- 2.3 Boundary Conditions
  - 2.3.1 Far field
  - 2.3.2 Viscous (smooth, rough, heat transfer, etc)
  - 2.3.3 Modeled boundary conditions (fan face, porous walls, etc)

3.0 CFD Solution Technology
- 3.1 General Comments
- 3.2 Classes of CFD technology: structured-grid, unstructured-grid, FEM….
- 3.3 Grid Generation
  - 3.3.1 General Comments
  - 3.3.2 Grid Generation Process
  - 3.3.3 Grid Structure
  - 3.3.4 Geometry
  - 3.3.5 Surface Grid Generation
  - 3.3.6 Volume Grid Generation
  - 3.3.7 Domain Connectivity
- 3.4 Algorithms
  - 3.4.1 General Comments
  - 3.4.2 Spatial Discretization
  - 3.4.3 Temporal Integration
  - 3.4.4 Spatial Integration
  - 3.4.5 Solution Adaption
- 3.5 Validation and Verification
  - 3.5.1 General Comments
  - 3.5.2 Code Validation and Verification
  - 3.5.3 Solution Verification
  - 3.5.4 Control of Errors

4.0 CFD Postprocessing
- 4.0.1 General Comments
- 4.0.2 Solution Evaluation
- 4.0.3 Sensitivity Studies
- 4.0.4 Interpretation
- 4.0.5 Knowledge Intrinsic/Endemic Limitations

Figure 3.- Governing Equations Extension

- 2.1 Governing Equations
  - 2.1.1 General Comments
  - 2.1.2 Panel Methods
  - 2.1.3 Transonic Small Disturbance (TSD)
  - 2.1.4 Potential
  - 2.1.5 Euler
  - 2.1.6 Reynolds Averaged Navier-Stokes (RANS)
    - 2.1.6.1 General Comments
    - 2.1.6.2 Physics Modeling
      - 2.1.6.2.1 Transition Modeling
        - 2.1.6.2.1.1 General Comments
        - 2.1.6.2.1.2 Trips
      - 2.1.6.2.2 Turbulence Modeling
        - 2.1.6.2.2.1 General Comments
        - 2.1.6.2.2.2 Linear Eddy-Viscosity Models
          - 2.1.6.2.2.2.1 The Boussinesq Approximation
          - 2.1.6.2.2.2.2 Algebraic Models
          - 2.1.6.2.2.2.3 ½Equation Models
          - 2.1.6.2.2.2.4 One Equation Models
          - 2.1.6.2.2.2.5 Two Equation Models
            - 2.1.6.2.2.2.5.1 K-ε Models
            - 2.1.6.2.2.2.5.2 K-ω Models
          - 2.1.6.2.2.2.6 Others
        - 2.1.6.2.2.3 Non-Linear Eddy Viscosity Models and Algebraic Stress Models
          - 2.1.6.2.2.3.1 Explicit Algebraic Stress Models
          - 2.1.6.2.2.3.2 Implicit Algebraic Stress Models
          - 2.1.6.2.2.3.3 Non-Linear Eddy Viscosity Models
        - 2.1.6.2.2.4 Differential Reynolds Stress Models
        - 2.1.6.2.2.5 Higher-Order Models
          - 2.1.6.2.2.5.1 Structure Function Model
      - 2.1.6.2.3 Finite-Rate Chemically Reacting Flows
    - 2.1.6.3 Algorithms
      - 2.1.6.3.1 Spatial Differencing
        - 2.1.6.3.1.1 Finite Difference
        - 2.1.6.3.1.2 Finite Volume
        - 2.1.6.3.1.3 Finite Element
      - 2.1.6.3.2 Temporal Integration
        - 2.1.6.3.2.1 Steady
          - 2.1.6.3.2.1.1 Explicit
            - 2.1.6.3.2.1.1.1 Runge-Kutta
          - 2.1.6.3.2.1.2 Implicit
            - 2.1.6.3.2.1.2.1 Approximate Factorization
            - 2.1.6.3.2.1.2.2 Line Gauss Seidel
            - 2.1.6.3.2.1.2.3 Symmetric Gauss-Seidel
        - 2.1.6.3.2.2 Unsteady
          - 2.1.6.3.2.2.1 Explicit
          - 2.1.6.3.2.2.2 Implicit
      - 2.1.6.3.3 Solution Adaption
        - 2.1.6.3.3.1 Feature Adaption
        - 2.1.6.3.3.2 Adjoint Based Adaption
  - 2.1.7 Parabolized Navier-Stokes (PNS)
  - 2.1.8 Unsteady Reynolds Averaged Navier-Stokes (URANS)
  - 2.1.9 Detached Eddy Simulation (DES)
  - 2.1.10 Large Eddy Simulation (LES)
  - 2.1.11 Sub-Grid Scale Models (SGS)
  - 2.1.12 Direct Numerical Simulation (DNS)
  - 2.1.13 Direct Simulation-Monte Carlo (DSMC)

Figure 4.- Grid Generation Extension

3.3 Grid Generation
- 3.3.1 General Comments
- 3.3.2 Grid Generation Process
- 3.3.3 Grid Structure
  - 3.3.3.1 Structured
    - 3.3.3.1.1 Single Block
    - 3.3.3.1.2 Multiblock
    - 3.3.3.1.3 Patched
    - 3.3.3.1.4 Overset
  - 3.3.3.2 Unstructured
    - 3.3.3.2.1 Tetrahedral
    - 3.3.3.2.2 General
  - 3.3.3.3 Hybrid

3.4 Geometry
- 3.4.1 Geometry Modeling Quality Issues
- 3.4.2 CAD Interface

3.5 Surface Grid Generation
- 3.5.1 Surface Grid Quality Issues

3.6 Volume Grid Generation
- 3.6.1 Volume Grid Quality Issues
  - 3.6.1.1 Cell Aspect Ratios
  - 3.6.1.2 Stretching
  - 3.6.1.3 Skewing
  - 3.6.1.4 Spacing of Near-Wall Points
  - 3.6.1.5 Pole Singularities

3.7 Domain Connectivity